Omega invariant of graphs and cyclicness

S. Delen, A. Yurttas, M. Togan, I. N. Cangul

Abstract. Starting with the formula for the number of leaves of a tree, two of the authors recently defined a new graph invariant called Omega denoted by $\Omega(G)$ only in terms of a given degree sequence. This invariant is shown to have many important combinatorial applications in graph theory and gives direct information compared to the better known Euler characteristic on the realizability, connectedness, cyclicness. Also some extremal problems are recently solved by means of it. In this paper, some new properties of Omega invariant, especially those related to the cyclicness and the number of components of the realized graphs are obtained.

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1 Introduction

We denote a graph with $\mid V(G) \mid = n$ vertices and $\mid E(G) \mid = m$ edges by $G = (V, E)$. Usually, the numbers n and m are called the order and size of G. For $v \in V(G)$, the degree of v will be denoted by d_v. A vertex of degree one is usually called a pendant vertex. We use the term "pendant edge" for an edge having a pendant vertex. The biggest vertex degree in a graph is often denoted by Δ. A graph is called connected if we can find a path between every pair of vertices, and disconnected otherwise.

Written with multiplicities, a degree sequence is written as

$$D(G) = \{{d_1}^{(a_1)}, {d_2}^{(a_2)}, {d_3}^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\},$$

where d_i's and a_i's are non-negative integers. It is also possible to state a degree sequence as

$$D(G) = \{0^{(a_0)}, 1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\},$$

where some of a_i's could be zero. Here $0^{(a_0)}$ means that there are a_0 isolated vertices and naturally in such a case, the graph is disconnected.

Let $D = \{d_1, d_2, d_3, \cdots, \Delta\}$ be a set of non-decreasing non-negative integers. We say that a graph G is a realization of the set D if the degree sequence of G is equal

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to D. In such a case, the set D will be called realizable.

It is clear from the definition that for a realizable degree sequence, there is at least one graph having this degree sequence. For example, the completely different two graphs in Figure 1 have the same degree sequence:

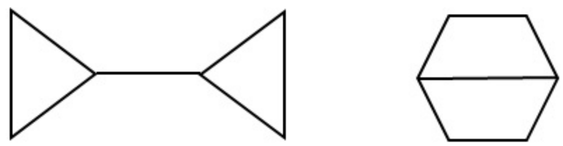

Figure 1 Graphs with the same DS

There are results to determine whether a given set is realizable or not, such as Havel-Hakimi, Erdös-Gallai, Ryser, Berge, Fulkerson-Hoffman-McAndrew, Bollobas, Grunbaum, Hasselbarth, Sierksma and Hoogeveen criteria, see [1], [2], [3], [4], [7], [8], [9], [10], [11], [12], [13]. Of course, the most basic criteria says that the sum of all vertex degrees must be even, as it is equal to twice the number of edges.

In many occasions, we classify our graphs under consideration according to whether they have at least one cycle or not. Those graphs having no cycle will be called acyclic. For example, all trees are acyclic. The remaining graphs are called cyclic graphs.

There are two special types of edges: An edge connecting a vertex to itself is called a loop, and at least two edges connecting two vertices are called multiple edges. When there are no loops nor multiple edges, then the graph is called simple.

Since 1980s, molecules are modelled as graphs by replacing atoms and chemical bonds with vertices and edges of the graph, respectively. We call this type of graph a molecular graph.

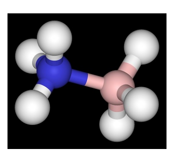

Figure 2 Ethane C_2H_6

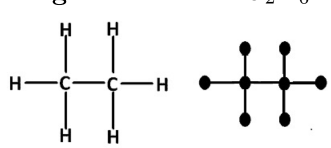

Figure 3 Graph corresponding to Ethane C_2H_6

When a situation is modelled by a graph, we can study this graph by mathematical methods to obtain several mathematical results. These mathematical results help us to comment on the properties of this situation. This means that easily calculated mathematical formulae are preferred over more geometric, electrostatic and chemical methods usually needing expensive laboratory equipments and a lot of time.

By means of mathematical models of chemical substances, we can calculate the boiling and melting points, molecular weights, atomic weights, density, branchedness, isomeration, reformation, spectroscopic properties and many other structural properties of atoms and molecules. We do these by means of some mathematical formulae called as topological graph indices.

The first topological graph index capable of characterizing the branchedness of alkanes was proposed by Wiener in 1947 to predict the boiling points of isomeric alkanes. The Wiener index was defined as the sum of the distances between any two carbon atoms in an alkane molecule and helped to order the isomers of alkanes according to their boiling points.

In this paper, we study several properties of graphs by means of recently defined mathematical formula which appears to be a topological graph invariant.

2 Omega invariant

First we recall from [5] the definition of this new graph invariant:

Definition 2.1. Let $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$ be the degree sequence of a graph G. The $\Omega(G)$ is defined only in terms of the degree sequence as

$$\begin{aligned}\Omega(G) = &\ a_3 + 2a_4 + 3a_5 + \cdots + (\Delta - 2)a_\Delta - a_1 \\ = &\ \sum_{i=1}^{\Delta}(i-2)a_i.\end{aligned}$$

Many properties of this invariant have just been obtained in [5] and [6]. For a given degree sequence, it has been shown that if $\Omega \leq -4$, then the graph is certainly disconnected, if $\Omega = -2$ and the graph is connected, then the graph is certainly acyclic, and if $\Omega \geq 0$ and the graph is connected, then the graph is certainly cyclic. If Ω is odd, we can directly say that the given degree sequence is not realizable. In [5], it has been shown that omega invariant can be stated in terms of the numbers of vertices and edges:

Theorem 2.1. *For any graph G,*

$$\Omega(G) = 2(m - n).$$

In that sense, the invariant Ω is related to the cyclomatic number.

It was also shown that Ω of a graph G is additive over the set of the components of G. Two of the most important properties of this new invariant has been given in [5] as follows:

Theorem 2.2. *The number r of faces in any realization G of a given degree sequence D is*

$$r = \frac{\Omega(D)}{2} + 1.$$

Corollary 2.3. *Let $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \cdots, \Delta^{(a_\Delta)}\}$ be realizable as a graph G with c components. The number r of faces of G is given by*

$$r = \frac{\Omega(G)}{2} + c.$$

Proof. As $\Omega(G)$ is additive, r is additive, too. By Theorem 2.2, we know

$$r(G_i) = \frac{\Omega(G_i)}{2} + 1 \Rightarrow \sum_{i=1}^{c} r(G_i) = \sum_{i=1}^{c} \frac{\Omega(G_i)}{2} + \sum_{i=1}^{c} 1$$

$$\Rightarrow r(G) = \frac{\Omega(G)}{2} + c.$$

□

We now obtain some new properties of this invariant:

Theorem 2.4. *Let D be a degree sequence and let G be a connected realization of it. If $\Omega(D) = -2$, then G is an acyclic graph, in other words, a tree.*

Proof. Let $\Omega(D) = -2$. By Theorem 2.2, we can say that the number of faces of G is $r = \frac{-2}{2} + 1 = 0$. That means that there are no faces in this arbitrary realization of D. Therefore any realization of D must be a tree. □

Another direct result of Theorem 2.2 is as follows:

Theorem 2.5. *Let D be a degree sequence and let G be a connected realization of it. If $\Omega(D) = 0$, then G is a unicyclic graph, in other words, it has only one face.*

Proof. Let $\Omega(D) = 0$. By Theorem 2.2, we can say that the number of faces of G is $r = \frac{0}{2} + 1 = 1$. That means that there is only one face in this arbitrary realization of D. Therefore any realization of D must be a unicyclic graph. □

The following can easily be obtained similarly:

Theorem 2.6. *Let D be a degree sequence and let G be a connected realization of it. If $\Omega(D) = 2$, then G is a bicyclic graph, in other words, a graph with two faces.*

Theorem 2.7. *Let D be a degree sequence and let G be a connected realization of it. If $\Omega(D) = 4$, then G is a tricyclic graph, in other words, a graph with three faces.*

This results can be generalized and a new result can be given for any required number of faces of any realization of a given arbitrary degree sequence.

The number of components is an important notion in the study of graphs. Especially, in the study of connectedness, we need to know that there is only one component. The following is a new relation between the number of components of any arbitrary realization of a given degree sequence and its omega invariant:

Corollary 2.8. *For each graph G, we have*

$$c \geq -\frac{\Omega(G)}{2}.$$

Equivalently,

$$c \geq n - m.$$

Proof. By Corollary 2.3, we know that $r = \frac{\Omega(G)}{2} + c$. Also by Theorem 2.1, we have $\Omega(G) = 2(m-n)$ implying that $r = m-n+c$. As the number of faces r is non-negative, we conclude that $c \geq n - m$, as required. □

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